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Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions

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Abstract

In this paper we develop a trigonometrically fitted predictor–corrector (P–C) scheme, which is based on the well-known two-step second-order Adams–Bashforth method (as predictor) and on the third-order Adams–Moulton method (as corrector). Numerical experiments show that the new trigonometrically fitted P–C method is substantially more efficient than widely used methods for the numerical solution of initial-value problems (IVPs) with oscillating solutions.

MSC: 65L05; 65L06

Keywords: Numerical solution; Initial-value problems (IVPs); Predictor–corrector methods; Trigonometric fitting; Multistep methods; Adams–Bashforth–Moulton methods

1. Introduction

In many areas of quantum mechanics, physical chemistry and chemical physics, celestial mechanics, electronics and elsewhere one can find equations of the form

$$\mathbf{y}'(\mathbf{x}) = \mathbf{f}(\mathbf{x}, \mathbf{y}), \quad \mathbf{y}(\mathbf{x_0}) = \mathbf{y_0} \tag{1}$$

(especially when their solution has oscillatory behavior) (see [6,8]).

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The last two decades much research has been done for the numerical solution of (1). For a complete review about the methods developed for the solution of (1) see [3,13,14,16], and references therein, as well as [4,10,15,19,20]. Most of the above methods are for second-order differential equations. The main characteristic of all the methods developed in the literature for the numerical solution of (1) is that they belong to the class of multistep and hybrid techniques.

Exponential and trigonometric fitting is one of the most useful ways for the construction of efficient methods for the numerical integration of first-order initial-value problems with oscillating or periodic solution. Lyche [7] had introduced this procedure. Raptis and Allison [11] have developed a Numerov-type exponentially fitted method for second-order differential equations. The numerical results obtained in [11] show that these fitted methods are much more efficient than Numerov's method for the solution of the Schrödinger-type equations. More recently, Van Daele and others [18] introduced trigonometric fitting to the, so-called, *r-Adams* methods, but the methodology described in [18] is quite different than the one we introduce here. Furthermore, we have extended trigonometric fitting to other types of P–C methods, like the explicit advanced step-point (EAS) methods (see [9]).

In this paper we will apply the procedure of trigonometric fitting for the construction of predictor–corrector methods for first-order initial-value problems with oscillating or periodic solution.

The paper is constructed as follows: In Section 2 the new trigonometrically fitted method is developed. In Section 3 the stability analysis is presented. Numerical illustrations are described in Section 4. Finally, in Section 5 we present the concluding remarks.

2. Trigonometrically fitted P–C methods

Consider the following well-known P–C scheme, which has also been used by Shampine and Gordon [12]:

$$\bar{y}_{n+1} = y_n + h\sum_{i=0}^{k-1} b_i \nabla^i f_n,$$

$$y_{n+1} = y_n + h\sum_{i=0}^{k} c_i \nabla^i \bar{f}_{n+1}. \tag{2}$$

Scheme (2) is designed so that the corrector is always one order higher than the predictor. From the above general case we can extract the following two-step scheme:

$$\bar{y}_{n+1} = y_n + h(b_0 f_n + b_1 f_{n-1}),$$

$$y_{n+1} = y_n + h(c_0 \bar{f}_{n+1} + c_1 f_n + c_2 f_{n-1}), \tag{3}$$

where b_i, $i = 0,1$ are the known Adams–Bashforth coefficients and the c_i, $i = 0,1,2$ coefficients correspond to the Adams–Moulton coefficients for both case (2) above, as well as for $w = 0$, see (7) below.

In order for the above method to be exact for any linear combination of the functions

$$\{1, x, \cos(\pm v\mathrm{x}), \sin(\pm v\mathrm{x})\} \tag{4}$$

the following system of equations must hold:

$$\begin{aligned}
&c_0 + c_1 + c_2 = 1,\\
&\cos(w) - 1 = -w^2(c_0 b_0 + c_0 b_1 \cos(w)) + c_2 w \cos(w),\\
&\sin(w) = w(c_0 + c_1 + c_2 \cos(w)) + w^2 c_0 b_1 \sin(w),
\end{aligned} \tag{5}$$

where $w = vh$. We note here that in the above system the first equation is produced from the requirement that method (3) is accurate for any linear combination of the functions $1, x$. The second and third equations are produced from the requirement that method (3) is accurate for any linear combination of the functions $\cos(\pm v x), \sin(\pm v x)$. The solution of this system of equations is given by

$$\begin{aligned}
c_0 &= \frac{1}{2}\,\frac{w - \sin(w) + w\cos(w)}{w^2 \sin(w)},\\
c_1 &= \frac{1}{4}\,\frac{w^2 + 3w^2\cos(2w) - 2\cos(w) + 2\cos(3w) + w\sin(3w) - 3w\sin(w) + 4w^2\cos(w)}{\cos(2w) - 1},\\
c_2 &= \frac{1}{4}\,\frac{-5w - 4w\cos(w) + w\cos(2w) + 7\sin(w) - \sin(3w) - 4w\sin(w)}{\cos(2w) - 1}.
\end{aligned} \tag{6}$$

For small values of w the above formulae are subject to heavy cancellations. In such a case the following Taylor series expansions should be used:

$$\begin{aligned}
c_0 &= \tfrac{5}{12} - \tfrac{31}{720} w^2 + \tfrac{41}{30240} w^4 - \tfrac{31}{1209600} w^6 + \tfrac{61}{239500800} w^8 - \tfrac{311}{118879488000} w^{10}\\
&\quad - \tfrac{1}{523069747200} w^{12} - \tfrac{4127}{10670622842880000} w^{14} + \cdots,\\
c_1 &= \tfrac{2}{3} - \tfrac{11}{240} w^2 + \tfrac{79}{30240} w^4 - \tfrac{97}{1209600} w^6 + \tfrac{73}{79833600} w^8 - \tfrac{21251}{1307674368000} w^{10}\\
&\quad - \tfrac{1}{9510359040} w^{12} - \tfrac{257}{47424990412800} w^{14} + \cdots,\\
c_2 &= -\tfrac{1}{12} + \tfrac{4}{45} w^2 - \tfrac{1}{252} w^4 + \tfrac{1}{9450} w^6 - \tfrac{1}{855360} w^8 + \tfrac{257}{13621608000} w^{10}\\
&\quad + \tfrac{1}{9340531200} w^{12} + \tfrac{11}{1894641840000} w^{14} + \cdots\ .
\end{aligned} \tag{7}$$

In Fig. 1 we present the behavior of the coefficients $c[i] = c_i,\ i = 0(1)2$, where $c_i,\ i = 0, 1, 2$ are given by (6). It is easy to see that for $6.2 < w < 6.4$ is better to use the Taylor series expansion.

The local truncation error of method (3) with coefficients given by (7) is equal to

$$\mathrm{LTE} = -\tfrac{1}{144} h^4 (6 y_n^{(4)} + 25 y_n^{(3)} - 19 w^2 y_n^{(2)}) + \mathrm{O}(h^5), \tag{8}$$

where $y_n^{(2)}$ is the second derivative of y at x_n, $y_n^{(3)}$ is the third derivative of y at x_n and $y_n^{(4)}$ is the fourth derivative of y at x_n. We note here that in order to produce Eq. (8) we express the quantities $y_{n+1},\ y_{n-1}$ and $f_{n+1},\ f_{n-1}$ around the point x_n and then we substitute the relevant expressions into (3).

It can be seen that when $v \to 0$ the above case (7) becomes the original predictor–corrector method of this type.

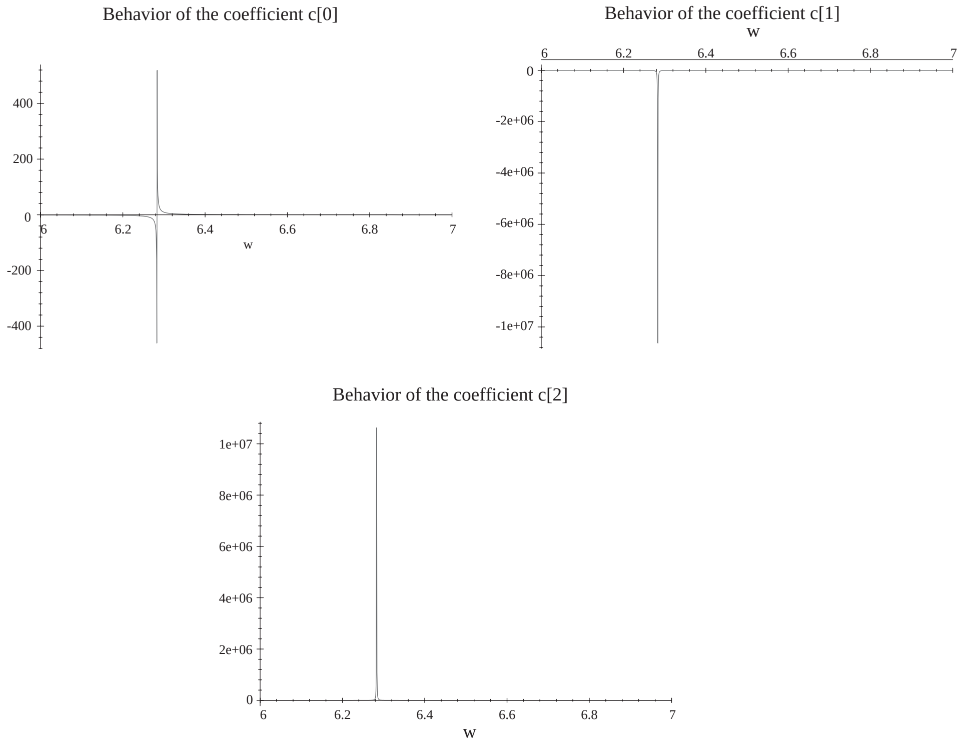

Fig. 1. Behavior of the coefficients c_i, $i = 0(1)2$ given by (6) for several values of v.

Following similar procedures, we can produce methods of the above type for multi-frequency cases, but this will be investigated in a future paper.

3. Stability analysis

Applying scheme (3) with coefficients $b_0 = \frac{3}{2}$ and $b_1 = -\frac{1}{2}$ to the scalar test equation

$$y' = \lambda y, \quad \text{where } \lambda \in \mathscr{C}, \tag{9}$$

we obtain the following difference equation:

$$y_{n+1} - A(H) y_n + B(H) y_{n-1} = 0, \tag{10}$$

where

$$A(H) = 1 + (c_0 + c_1)H + \frac{3}{2} c_0 H^2, \quad B(H) = \frac{H}{2}(2c_2 + c_0 H). \tag{11}$$

The characteristic equation of (10) is given by

$$r^2 - A(H) r + B(H) = 0. \tag{12}$$

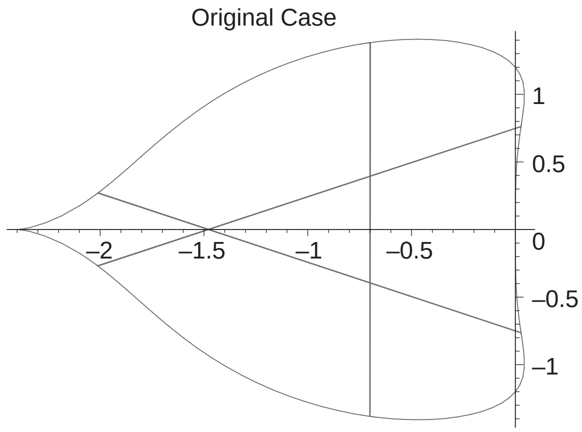

Fig. 2. Stability region for the original case.

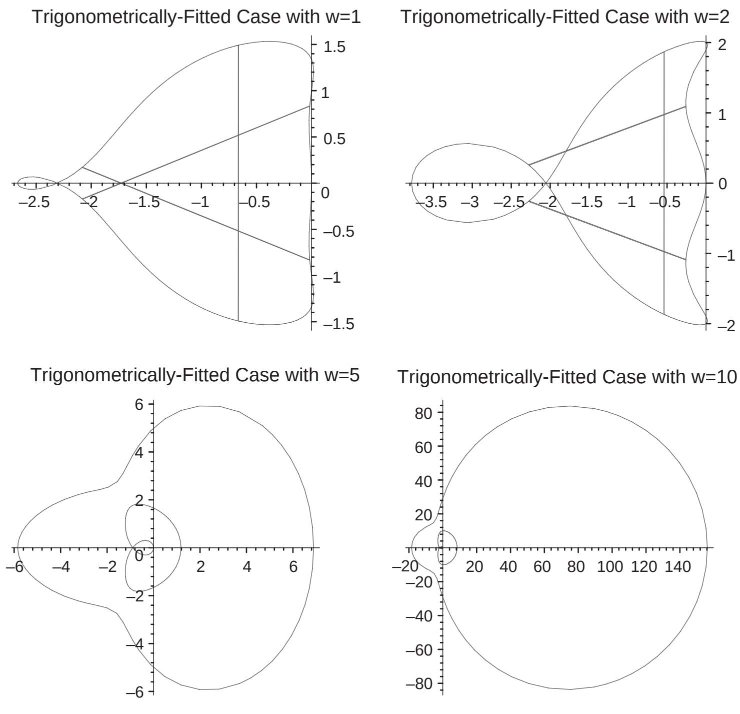

Fig. 3. Stability region for the trigonometrically fitted case and for $w = 1$ (above left), $w = 2$ (above right), $w = 5$ (below left) and $w = 10$ (below right).

Using the boundary locus technique [5] by solving the above equation in H and substituting $r = \exp(i\theta)$, where $i = \sqrt{-1}$, we can plot the regions of absolute stability for $\theta \in [0, 2\pi]$. In Fig. 2 we present the region of absolute stability for the original case (i.e., method (3) without trigonometric fitting). In Fig. 3 we present the region of absolute stability for the trigonometrically fitted case and for $w = 1$, 2, 5 and 10. It should be noted in Fig. 3 that the larger the frequency w, the larger the region of absolute stability.

4. Numerical illustrations

In this section we apply the new method to three problems: the first is an inhomogeneous equation, the second is the Stiefel and Bettis orbit problem [17] and the third is the Duffing's equation.

In all our numerical illustrations, we compare the following methods:

(I) The original predictor–corrector method given by (3), i.e., method (3) without trigonometric fitting, is indicated as Method (a).

(II) The well-known predictor–corrector Adams–Bashforth–Moulton method of algebraic order four is indicated as Method (b). (Note that, besides the lower order, a further difference between Method (a) and Method (b) is that Method (b) is designed so that the order of the corrector is the same as the order of the predictor. In other words, this is a different type of P–C method.)

(III) The classical fourth algebraic order Runge–Kutta method [2] is indicated as Method (c).

(IV) The new trigonometrically fitted predictor–corrector third algebraic order two-step method is indicated as Method (d).

4.1. Inhomogeneous equation

We consider the following problem:

$$y'' = -100y + 99\sin(x), \quad y(0) = 1, \quad y'(0) = 11 \tag{13}$$

which has a solution of the form $y(x) = \cos(10x) + \sin(10x) + \sin x$.

Eq. (13) has been solved numerically for $0 \leqslant x \leqslant 40\pi$ and with $w = 10$ using the aforementioned methods.

In Fig. 4 we present the maximum absolute error of the four methods for the inhomogeneous Eq. (13). The absence of values for $\mathrm{Err}_{\max}$ for Methods (a)–(c) indicate that for such number of function evaluations, the values of $\mathrm{Error}_{\max}$ are not accepted, i.e., they are positive:

$$\mathrm{Err}_{\max} = \log_{10}\left(\max_{0\leqslant x\leqslant 40\pi} |y_{\text{calculated}}(x) - y_{\text{theoretical}}(x)|\right) \tag{14}$$

for the same number of function evaluations (NFE), which are equal to NFE $\times$ 100 (where NFE is the value on the axis of x on the diagram and this value on the x-axis is equal to NFE $\times$ 100).

4.2. Duffing's equation

Considered the Duffin's equation:

$$y'' + y + y^3 = B\cos(\omega x), \quad y(0) = A_1 + A_3 + A_5 + A_7, \quad y'(0) = 0 \tag{15}$$

with a solution of the form

$$y(x) = \sum_{i=0}^{3} A_{2i+1}\cos[(2i+1)\omega x], \tag{16}$$

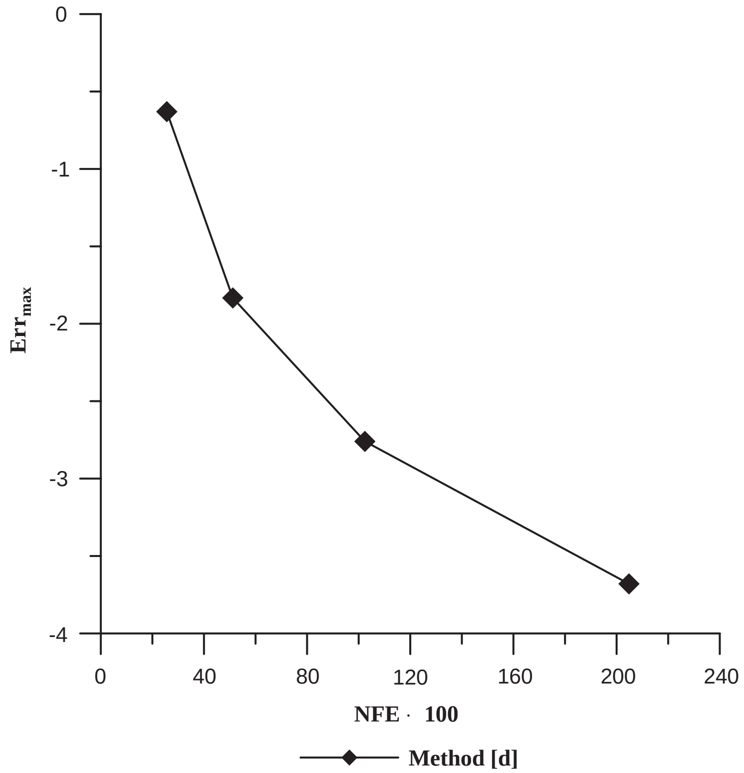

Fig. 4. Values of $\mathrm{Err}_{\max}$ for several values of NFE × 100 for the inhomogeneous equation. —◆—, Method (d).

where

$$B = 0.002, \quad \omega = 1.01, \quad A_1 = 0.200179477536,$$
$$A_3 = 0.246946143 \times 10^{-3}, \quad A_5 = 0.304016 \times 10^{-6}, \quad A_7 = 0.347 \times 10^{-9}. \tag{17}$$

Eq. (15) has been solved numerically for $0 \leqslant x \leqslant 40\pi$ and $w = 1$ using the above mentioned methods.

In Fig. 5 we present the maximum absolute error (14) for the same number of function evaluations which are equal to NFE × 100.

4.3. *Stiefel and Bettis problem [17]*

Consider the system of equations:

$$y'' + y = 0.001\cos(x),$$
$$z'' + z = 0.001\sin(x) \tag{18}$$

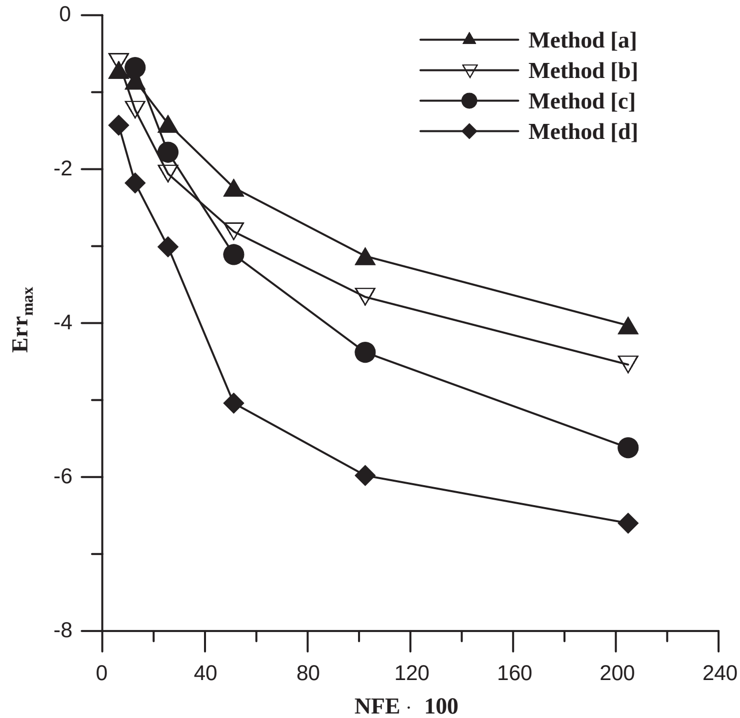

Fig. 5. Values of Err_{max} for several values of NFE $\times$ 100 for the Duffing's equation: —▲—, Method (a); —▽—, Method (b); —•—, Method (c); —♦—, Method (d).

with initial conditions

$$y(0) = 1, \quad y'(0) = 0, \quad z(0) = 0, \quad z'(0) = 0.9995. \tag{19}$$

The analytical solution of the above problem is given by

$$y(x) = \cos(x) + 0.0005x\sin(x),$$
$$z(x) = \sin(x) - 0.0005x\cos(x). \tag{20}$$

Problem (18) has been solved numerically for $0 \leqslant x \leqslant 40\pi$ and $w = 1$ using the above-mentioned methods.

In Fig. 6 we present the maximum absolute error (14) for the same number of function evaluations which are equal to NFE $\times$ 100.

5. Remarks and conclusion

For all the problems the new trigonometrically fitted method is much more efficient than the other methods. For the inhomogeneous equation all methods, except the new one, are diverging. For Duffing's equation the known fourth-order Runge–Kutta method is more efficient than the P–C

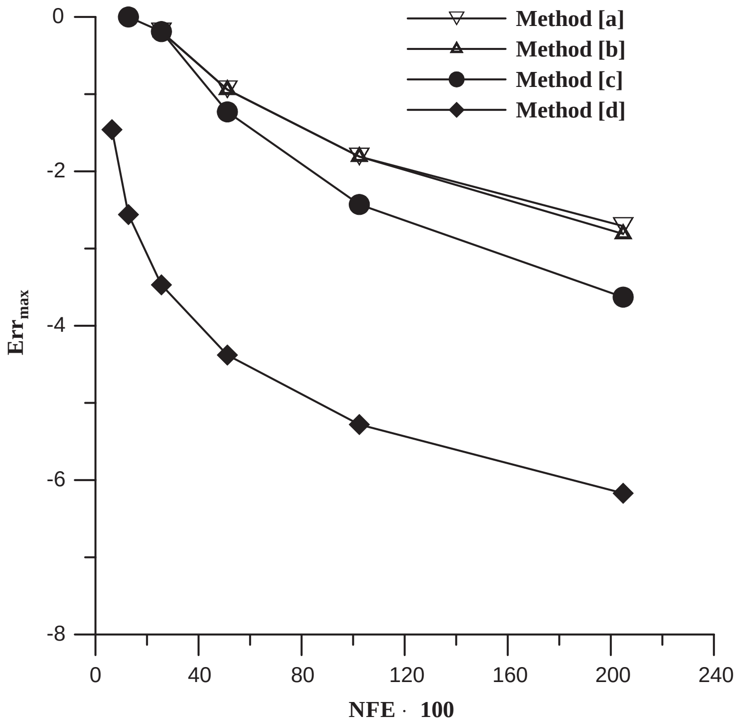

Fig. 6. Values of Err_{max} for several values of NFE × 100 for the Stiefel and Bettis problem: —▽—, Method (a); —▲—, Method (b); —•—, Method (c); —♦—, Method (d).

fourth-order Adams–Bashforth–Moulton method. This last Adams–Bashforth–Moulton P–C method is more efficient than method (3) with constant coefficients.

Finally, for the Stiefel and Bettis problem [17], the behavior of the original (nontrigonometrically fitted) method (3) is very similar to the P–C fourth algebraic order Adams–Bashforth–Moulton method. But it behaves worse compared to the classical fourth algebraic order Runge–Kutta method.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

6. Uncited reference

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